# STAT 542: Statistical Learning <br> Logistic Regression and Discriminant Analysis 

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## Outline

- Classification problems
- Logistic Regression
- Evaluating Classification Models
- LDA and QDA
- Remarks


## Classification Problems

- Training data $\mathcal{D}_{n}=\left\{x_{i}, y_{i}\right\}_{i=1}^{n}$ :

$$
\text { - } x_{i} \in \mathbf{R}^{p} \text {, and } y_{i} \in\{0,1\} \text { (sometimes we use }\{-1,+1\} \text { ). }
$$

- The goal is to find a classifier

$$
f: \mathbf{R}^{p} \longrightarrow\{0,1\}
$$

- At any target point $x$ with outcome $y$, the performance of a classifier is usually measured by $0-1$ loss

$$
L(f(x), y)=\left\{\begin{array}{lll}
0 & \text { if } & y=f(x) \\
1 & \text { if } & \text { o.w. }
\end{array}\right.
$$

## Soft vs. Hard Classification

- There are two popular approaches when modeling binary data
- Soft classifiers
- Estimate the conditional probabilities $P(Y \mid X)$
- Use $1\{P(Y \mid X)>c\}$ for classification
- e.g. logistic regression
- Hard classifiers
- Directly estimate the classification decision boundary
- e.g. svm
- Many methods are capable of doing or have been extended to perform both


## Logistic Regression

## Motivation

- Directly model the probability

$$
\eta(x)=\mathrm{P}(Y=1 \mid X=x)
$$

- $\eta(x)$ should be bounded within $[0,1]$
- Consider a link function $g$ that transform $\eta(x)$ into $(-\infty, \infty)$, then

$$
g(\eta(x))=x^{\top} \beta
$$

- Generalized linear model (GLM)


## Motivation

- Response $Y$ follows a Bernoulli distribution conditioning on $x$ :

$$
p\left(Y=y_{i} \mid X=x_{i}\right)=\eta\left(x_{i}\right)^{y_{i}}\left[1-\eta\left(x_{i}\right)\right]^{1-y_{i}}
$$

- For Logistic regression, we use the logit link function

$$
\log \frac{\eta(x)}{1-\eta(x)}=x^{\top} \beta, \quad \eta(x)=\frac{\exp \left(x^{\top} \beta\right)}{1+\exp \left(x^{\top} \beta\right)}
$$

- $\log \frac{p}{1-p}$ is called log-odds, and we are modeling it as a linear function of $x$.


## Fitting Logistic Models

- Maximize the log-likelihood function, using the conditional likelihood of $Y$ given $X$ :

$$
\begin{aligned}
\ell(\boldsymbol{\beta}) & =\sum_{i=1}^{n} \log p\left(y_{i} \mid x_{i}, \boldsymbol{\beta}\right) \\
& =\sum_{i=1}^{n} \log \left\{\eta\left(x_{i}\right)^{y_{i}}\left[1-\eta\left(x_{i}\right)\right]^{1-y_{i}}\right\} \\
& =\sum_{i=1}^{n} y_{i} \log \frac{\eta\left(x_{i}\right)}{1-\eta\left(x_{i}\right)}+\log \left[1-\eta\left(x_{i}\right)\right] \\
& =\sum_{i=1}^{n} y_{i} x_{i}^{\top} \boldsymbol{\beta}-\log \left[1+\exp \left(x_{i}^{\top} \boldsymbol{\beta}\right)\right]
\end{aligned}
$$

## Newton-Raphson

- Derive the first and second derivatives
- Use Newton's method to update $\beta$ by

$$
\boldsymbol{\beta}^{\text {new }}=\boldsymbol{\beta}^{\text {old }}-\left.\left[\frac{\partial^{2} \ell(\boldsymbol{\beta})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^{\top}}\right]^{-1} \frac{\partial \ell(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}}\right|_{\boldsymbol{\beta}^{\text {old }}}
$$

where

$$
\begin{aligned}
& \text { (gradient) } \frac{\partial \ell(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}}=\sum_{i=1}^{n} y_{i} x_{i}^{\top}-\sum_{i=1}^{n} \frac{\exp \left(x_{i}^{\top} \boldsymbol{\beta}\right) x_{i}^{\top}}{1+\exp \left(x_{i}^{\top} \boldsymbol{\beta}\right)} \\
& \text { (Hessian) }
\end{aligned} \frac{\partial^{2} \ell(\boldsymbol{\beta})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^{\top}}=-\sum_{i=1}^{n} x_{i} x_{i}^{\top} \eta\left(x_{i}\right)\left[1-\eta\left(x_{i}\right)\right], ~ l
$$

## Interpreting Parameters

- What is the effect of $\beta$ ?
- Wrong:
- Each unit increases of $X_{j}$ increases the probability of $Y$ by $\boldsymbol{\beta}_{j}$
- Correct:
- Each unit increases of $X_{j}$ increases the log-odds of $Y$ by $\boldsymbol{\beta}_{j}$


## Evaluating Classification

 Models
## Correct or Wrong decision?

- In hypothesis testing problems, we have the following $2 \times 2$ table:

|  | Accept $H_{0}$ | Reject $H_{0}$ |
| :---: | :---: | :---: |
| $H_{0}$ true | $\checkmark$ | Type I Error |
| $H_{0}$ false | Type II Error | $\checkmark$ |

- For classification problems, we face the same decision problems
- Instead of using the $\alpha$-level (to tune), we can use different thresholds on $P(Y \mid X)$ to make the decision.


## A Motivating Example

- A new lab test is developed for detecting Covid-19 infection based on the score obtained from a device
- If the test returns positive (the score is larger than a threshold $c$ ), then we conclude infection.
- If the test returns negative (the score is lower than $c$ ), we conclude no infection.
- We collect the following data from 1000 tests

|  | Infection | No Infection |  |
| :---: | :---: | :---: | :---: |
| Test Positive | 20 | 70 | 90 |
| Test Negative | 10 | 900 | 910 |
|  | 30 | 970 | 1000 |

## Confusion Matrix

|  | Infection | No Infection |
| :---: | :---: | :---: |
| Test Positive | True Positive <br> (TP) | False Positive <br> (FP, Type I Error) |
| Test Negative | False Negative <br> (FN, Type II Error) | True Negative <br> (TN) |

- One way to evaluate this model (test) is the overall accuracy

$$
\begin{aligned}
\text { Overall Accuracy } & =\frac{\text { All Correct Decisions }}{\text { All Decisions }} \\
& =\frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}
\end{aligned}
$$

- However, this is not always good, especially when we have unbalanced data


## Overall Accuracy

- Sometimes we can simply use the overall accuracy:

$$
\begin{aligned}
\text { Overall Accuracy } & =\frac{\text { All Correct Decisions }}{\text { All Decisions }} \\
& =\frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}
\end{aligned}
$$

|  | Infection | No Infection |
| :---: | :---: | :---: |
| Test Positive | TP | FP |
| Test Negative | FN | TN |

- In our Trisomy test data, the overall accuracy is $92 \%$.
- However, accuracy may not be very informative.


## Sensitivity and Specificity

- Sensitivity (also called "Recall") is the defined as the true positive rate (among the infected population, what proportion are correctly identified by the test)

$$
\text { Sensitivity }=\frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}
$$

|  | Infection | No Infection |
| :---: | :---: | :---: |
| Test Positive | TP | FP |
| Test Negative | FN | TN |

- In our data, the sensitivity is $\frac{20}{20+10} \approx 66.7 \%$


## Sensitivity and Specificity

- Specificity is the defined as the true negative rate (among the non-trisomy population, what proportion are correctly identified by the test)

$$
\text { Specificity }=\frac{\mathrm{TN}}{\mathrm{TN}+\mathrm{FP}}
$$

|  | Infection | No Infection |
| :---: | :---: | :---: |
| Test Positive | TP | FP |
| Test Negative | FN | TN |

- In our data, the specificity is $\frac{900}{900+70} \approx 92.8 \%$


## ROC Curve

- However, we can also alter the decision threshold $c$, which leads to a different sensitivity and specificity combination
- As we alter the threshold, the two measures form an ROC (receiver operating characteristic) curve
- $x$-axis: 1 - Specificity: False Positive Rate
- $y$-axis: Sensitively: True Negative Rate



## LDA and QDA

## Motivation: Bayes Rule

- Recall that if we use the $0-1$ loss as the criteria

$$
L(f(x), y)=\left\{\begin{array}{lll}
0 & \text { if } & y=f(x) \\
1 & \text { if } & \text { o.w. }
\end{array}\right.
$$

- Then, the best rule we can get is

$$
f_{B}(x)=\underset{f}{\arg \min } \mathrm{R}(f)=\left\{\begin{array}{lll}
1 & \text { if } & \eta(x)>1 / 2 \\
0 & \text { if } & \eta(x)<1 / 2
\end{array}\right.
$$

- This rule $f_{B}$ is called the Bayes rule, and the corresponding risk (expected loss) is the Bayes risk or Bayes error.


## Motivation: Bayes Rule

- The name of "Bayes rule" comes from understanding the optimal rule from the Bayes prospective:

$$
\begin{aligned}
& \mathrm{P}(Y=1 \mid X=x)=\frac{\mathrm{P}(X=x \mid Y=1) \mathrm{P}(Y=1)}{\mathrm{P}(X=x)} \\
& \mathrm{P}(Y=0 \mid X=x)=\frac{\mathrm{P}(X=x \mid Y=0) \mathrm{P}(Y=0)}{\mathrm{P}(X=x)}
\end{aligned}
$$

## Bayes Rule

- Treating $\pi=\mathrm{P}(Y=1)$ and $(1-\pi)=\mathrm{P}(Y=0)$ as prior probabilities, and define the conditional densities of $X$ as

$$
f_{1}=\mathrm{P}(X=x \mid Y=1) \text { and } f_{0}=\mathrm{P}(X=x \mid Y=0)
$$

- The Bayes rule can also be written as

$$
f_{B}(x)=\underset{f}{\arg \min } \quad \mathrm{R}(f)=\left\{\begin{array}{lll}
1 & \text { if } & \pi f_{1}(x)>(1-\pi) f_{0}(x) \\
0 & \text { if } & \pi f_{1}(x)<(1-\pi) f_{0}(x) .
\end{array}\right.
$$

- Note that the marginal density of $X$ can also be written as

$$
\mathrm{P}(X=x)=\pi f_{1}(x)+(1-\pi) f_{0}(x)
$$

although it does not play a role in the optimal decision rule.

## Bayes Rule

- The prior probabilities: $\mathrm{P}(Y=0)$ and $\mathrm{P}(Y=1)$
- Reflect the prior knowledge of the likelihood of occurrence for each class
- Can be used to make a decision without any extra knowledge
- The posterior probabilities: $\mathrm{P}(Y \mid X)$
- The updated probabilities after observing $X=x$
- The Bayes decision rule combines them to achieve the minimum risk

$$
f_{B}(x)=1 \text { if } \frac{f_{1}(x)}{f_{0}(x)}>\frac{1-\pi}{\pi} ; \text { and } 0 \text { o.w. }
$$

## Bayes Rule

- The decision boundary can also be used to describe the optimal rule:

$$
\left\{x: \pi f_{1}(x)=(1-\pi) f_{0}(x)\right\}
$$

- Linear methods for classification: the classification rules with $f_{B}(x)$ being linear in $x$, or equivalently, classification rules with linear decision boundaries.


## Multi-Class Problems

- In multi-class problems, $y \in\{1, \ldots K\}$. We want to construct classifier

$$
f: \mathbf{R}^{p} \longrightarrow\{1, \ldots, K\}
$$

- The optimal rule is

$$
f_{B}(x)=\underset{k}{\arg \max } \mathbf{P}(Y=k \mid X=x)=\underset{k}{\arg \max } \pi_{k} f_{k}(x)
$$

where $\pi_{k}$ is prior probability and $f_{k}(x)$ is the conditional density for class $k$.

- Classify $x$ to the most probable class by comparing $\mathrm{P}(Y \mid X=x)$.


## Binary vs. Multi-Class

- We will focus on binary classifiers. Some binary classifiers can also handel multi-classes, such as discriminate analysis (LDA, QDA, NB), logistic regression, $k \mathrm{NN}$ and random forests. But for some others, the extension is non-trivial (SVM).
- There are some naive (although may not be optimal) ways to apply a binary classifier on a classification problem with $K>2$ categories.
- Train $K$ one-vs-other classifiers
- Train $K(K-1) / 2$ pairwise classifiers

Then we can combine the results to get a consensus prediction.

## Masking Problems in Linear Models

- For outcome $Y$, which may fall into categories $1, \ldots, K$, define a vector of indicators $\left(Y_{1}, \ldots, Y_{K}\right)$

$$
Y_{k}=1 \quad \text { if } \quad Y=k
$$

- Each vector $\left(Y_{1}, \ldots, Y_{K}\right)$ has a single 1.
- The $n$ training samples form an $n \times K$ indicator response matrix $\mathbf{Y}$, where each row is such an indicator vector.
- If we model each $Y_{k}$ separately, then this is essentially one-vs-other
- However, we may face serious masking problems


## Masking Problems

Fitting the three-class problem using polynomials


Degree = 1; Error = 0.33


Degree $=2$, Error $=0.04$

Note: LDA can avoid this problem

## Discriminant Analysis

## Linear Discriminant Analysis

- The idea is to model the distribution of $X$ in each of the classes separately, and then use Bayes theorem to flip things around and obtain $\mathrm{P}(Y \mid X=x)$.
- Linear Discriminant Analysis (LDA)
- Quadratic Discriminant Analysis (LDA)
- Naive Bayes (NB)


## Bayes Theorem for Classification

- As we demonstrated earlier (Bayes rules), the conditional probability can be formulated using Bayes Theorem:

$$
\begin{aligned}
\mathrm{P}(Y=k \mid X=x) & =\frac{\mathbf{P}(X=x \mid Y=k) \mathrm{P}(Y=k)}{\mathrm{P}(X=x)} \\
& =\frac{\mathrm{P}(X=x \mid Y=k) \mathrm{P}(Y=k)}{\sum_{l=1}^{K} \mathrm{P}(X=x \mid Y=l) \mathrm{P}(Y=l)} \\
& =\frac{\pi_{k} f_{k}(x)}{\sum_{l=1}^{K} \pi_{l} f_{l}(x)}
\end{aligned}
$$

where $f_{k}(x)$ is the conditional density function of $X \mid Y=k$, and $\pi_{k}=\mathrm{P}(Y=k)$ is the prior probability.

## Bayes Theorem for Classification

- The best prediction is picking the one that maximizing the posterior

```
arg max }\mp@subsup{\pi}{k}{}\mp@subsup{f}{k}{}(x
    k
```

- LDA and QDA model $f_{k}(x)$ as a normal distribution


## Bayes Theorem for Classification

- Suppose we model each class density as multivariate Gaussian $\mathcal{N}\left(\boldsymbol{\mu}_{k}, \Sigma_{k}\right)$, and assume that the covariance matrices are the same across all $k$, i.e., $\Sigma_{k}=\Sigma$. Then the

$$
f_{k}(x)=\frac{1}{(2 \pi)^{p / 2}|\Sigma|^{1 / 2}} \exp \left[-\frac{1}{2}\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma^{-1}\left(x-\boldsymbol{\mu}_{k}\right)\right]
$$

- The log-likelihood function for the conditional distribution is

$$
\begin{aligned}
\log f_{k}(x) & =-\log \left((2 \pi)^{p / 2}|\Sigma|^{1 / 2}\right)-\frac{1}{2}\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma^{-1}\left(x-\boldsymbol{\mu}_{k}\right) \\
& =-\frac{1}{2}\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma^{-1}\left(x-\boldsymbol{\mu}_{k}\right)+\text { constant }
\end{aligned}
$$

## Bayes Theorem for Classification

- Hence we just need to select the category that attains the highest posterior density (MAP: maximum a posteriori):

$$
\begin{aligned}
\widehat{f}(x) & =\underset{k}{\arg \max } \log \left(\pi_{k} f_{k}(x)\right) \\
& =\underset{k}{\arg \max }-\frac{1}{2}\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma^{-1}\left(x-\boldsymbol{\mu}_{k}\right)+\log \left(\pi_{k}\right)
\end{aligned}
$$

## Interpretations of LDA

- The term $\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma^{-1}\left(x-\boldsymbol{\mu}_{k}\right)$ is simply the Mahalanobis distance between $x$ and the centroid $\boldsymbol{\mu}_{k}$ for class $k$
- Classify $x$ to the class with the closest centroid (after adjusting the for prior)
- Special case: $\Sigma=\mathbf{I}$ (only Euclidean distance is needed)

$$
\underset{k}{\arg \max }-\frac{1}{2}\left\|x-\boldsymbol{\mu}_{k}\right\|^{2}+\log \left(\pi_{k}\right)
$$

## Decision Boundary

- Noticing that that quadratic term can be simplified to

$$
\begin{aligned}
& -\frac{1}{2}\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma^{-1}\left(x-\boldsymbol{\mu}_{k}\right) \\
= & x^{\top} \Sigma^{-1} \boldsymbol{\mu}_{k}-\frac{1}{2} \boldsymbol{\mu}_{k}^{\top} \Sigma^{-1} \boldsymbol{\mu}_{k}+\text { irrelevant things }
\end{aligned}
$$

- Then the discriminant function is defined as

$$
\begin{aligned}
\delta_{k}(x) & =x^{\top} \Sigma^{-1} \boldsymbol{\mu}_{k}-\frac{1}{2} \boldsymbol{\mu}_{k}^{\top} \Sigma^{-1} \boldsymbol{\mu}_{k}+\log \pi_{k} \\
& =\mathbf{w}_{k}^{\top} x+b_{k},
\end{aligned}
$$

- We can calculate $\mathbf{w}_{k}$ 's and $b_{k}$ 's for each class $k$ from the data.


## Decision Boundary

- The decision boundary function between class $k$ and $l$ is

$$
\begin{array}{ll} 
& \mathbf{w}_{k}^{\top} x+b_{k}=\mathbf{w}_{l}^{\top} x+b_{l} \\
\Leftrightarrow & \left(\mathbf{w}_{k}-\mathbf{w}_{l}\right)^{\top} x+\left(b_{k}-b_{l}\right)=0 \\
\Leftrightarrow & \widetilde{\mathbf{w}}^{\top} x+\widetilde{b}=0
\end{array}
$$

- Since $\mathbf{w}_{k}=\Sigma^{-1} \boldsymbol{\mu}_{k}$ and $\mathbf{w}_{l}=\Sigma^{-1} \boldsymbol{\mu}_{l}$, the decision boundary has the directional vector

$$
\widetilde{\mathbf{w}}=\Sigma^{-1}\left(\boldsymbol{\mu}_{k}-\boldsymbol{\mu}_{l}\right)
$$

## Interpretations of LDA



FIGURE 4.9. Although the line joining the centroids defines the direction of greatest centroid spread, the projected data overlap because of the covariance (left panel). The discriminant direction minimizes this overlap for Gaussian data (right panel).

## Parameter Estimations in LDA

- We estimate the LDA parameters from the training data
- Prior probabilities: $\widehat{\pi}_{k}=n_{k} / n=n^{-1} \sum_{k} \mathbf{1}\left\{y_{i}=k\right\}$, where $n_{k}$ is the number of observations in class $k$.
- Centroid: $\widehat{\mu}_{k}=n_{k}^{-1} \sum_{i: y_{i}=k} x_{i}$
- Pooled covariance:

$$
\widehat{\Sigma}=\frac{1}{n-K} \sum_{k=1}^{K} \sum_{i: y_{i}=k}\left(x_{i}-\widehat{\boldsymbol{\mu}}_{k}\right)\left(x_{i}-\widehat{\boldsymbol{\mu}}_{k}\right)^{\top}
$$

## Quadratic Discriminant Analysis

- Quadratic Discriminant Analysis simply abandons the assumption of the common covariance matrix. Hence, $\Sigma_{k}$ 's are not equal.
- In this case, the determinant $\left|\Sigma_{k}\right|$ of each covariance matrix will be different. The MAP decision becomes

$$
\begin{aligned}
& \max _{k} \log \left(\pi_{k} f_{k}(x)\right) \\
= & \max _{k}-\frac{1}{2} \log \left|\Sigma_{k}\right|-\frac{1}{2}\left(x-\boldsymbol{\mu}_{k}\right)^{\top} \Sigma_{k}^{-1}\left(x-\boldsymbol{\mu}_{k}\right)+\log \left(\pi_{k}\right) \\
= & x^{\top} \mathbf{W}_{k} x+\mathbf{w}_{k}^{\top} x+b_{k}
\end{aligned}
$$

- This leads to quadratic decision boundary between class $k$ and $l$

$$
\left\{x: x^{\top}\left(\mathbf{W}_{k}-\mathbf{W}_{l}\right) x+\left(\mathbf{w}_{k}^{\top}-\mathbf{w}_{l}^{\top}\right)^{\top} x+\left(b_{k}-b_{l}\right)=0\right\}
$$

## Estimations in QDA

- We estimate the QDA parameters from the training data
- Prior probabilities: $\widehat{\pi}_{k}=n_{k} / n=n^{-1} \sum_{k} \mathbf{1}\left\{y_{i}=k\right\}$, where $n_{k}$ is the number of observations in class $k$.
- Centroid: $\widehat{\boldsymbol{\mu}}_{k}=n_{k}^{-1} \sum_{i: y_{i}=k} x_{i}$
- Sample covariance matrix for each class:

$$
\widehat{\Sigma}_{k}=\frac{1}{n_{k}-1} \sum_{i: y_{i}=k}\left(x_{i}-\widehat{\boldsymbol{\mu}}_{k}\right)\left(x_{i}-\widehat{\boldsymbol{\mu}}_{k}\right)^{\top}
$$

## LDA vs. QDA

- More parameters in QDA than LDA, especially when $p$ is large
- Both are extremely simple to implement
- Both LDA and QDA can perform well on real classification problems
- We can include selected quadratic terms of the covariates, such as $X_{1} X_{2}$ or $X_{1}^{2}$, and still perform LDA


## LDA vs. QDA



FIGURE 4.6. Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using $L D A$ in the five-dimensional space $\left.X_{1}, X_{2}, X_{1} X_{2}, X_{1}^{2}, X_{2}^{2}\right)$. The right plot shows the quadratic decision boundaries found by $Q D A$. The differences are small, as is usually the case.

## Alternative Formulations

## Fisher's Criterion

- The between-class variation on those $K$ centroid $\left(\boldsymbol{\mu}_{1}, \ldots \boldsymbol{\mu}_{K}\right)$ is

$$
\begin{aligned}
& \qquad \begin{aligned}
\mathbf{B} & =\sum_{k=1}^{K} \pi_{k}\left(\boldsymbol{\mu}_{k}-\overline{\boldsymbol{\mu}}\right)\left(\boldsymbol{\mu}_{k}-\overline{\boldsymbol{\mu}}\right)^{\top} \\
\text { where } \quad \overline{\boldsymbol{\mu}} & =\sum_{k=1}^{K} \pi_{k} \boldsymbol{\mu}_{k}
\end{aligned} \text {. }
\end{aligned}
$$

- The within-class variation is just the common covariance matrix $\Sigma$ that we calculated in LDA, denote it as $\mathbf{W}$.
- If we define a linear combination $Z=a^{\top} X$ such that we want the between-class variance is maximized relative to the within-class variance, we maximize the Rayleigh quotient,

$$
\underset{a}{\operatorname{maximize}} \frac{a^{\top} \mathbf{B} a}{a^{\top} \mathbf{W} a} \quad \text { subject to } \quad a^{\top} \mathbf{W} a=1
$$

## Fisher's Criterion

- To solve this, note that $\mathbf{W}$ has to be positive definite (for sufficient large $n$ ), we write $\mathbf{W}=\left(\mathbf{W}^{\frac{1}{2}}\right)^{\top} \mathbf{W}^{\frac{1}{2}}$
- Define $b=\mathbf{W}^{\frac{1}{2}} a$, then $a=\mathbf{W}^{-\frac{1}{2}} b$, and the optimization problem becomes

$$
\underset{b}{\operatorname{maximize}} \frac{b^{\top}\left(\mathbf{W}^{-\frac{1}{2}}\right)^{\top} \mathbf{B} \mathbf{W}^{-\frac{1}{2}} b}{b^{\top} b} \text { subject to } \quad b^{\top} b=1
$$

- The maximizer is simply the first eigenvector of $\left(\mathbf{W}^{-\frac{1}{2}}\right)^{\top} \mathbf{B} \mathbf{W}^{-\frac{1}{2}}$.
- Recover $a=\mathbf{W}^{-\frac{1}{2}} b$, which is the first eigenvector of $\mathbf{W}^{-1} \mathbf{B}$.
- Similarly, one can find the next direction by extracting the second eigenvector.


## Reduced Rank LDA

- Low-dimensional structure of the data may help reduce the noise
- We may consider many different ways to reduced the rank of the data, and perform discriminant analysis on the dimensionality reduced space.
- Example 1 (a simple reduced-rank LDA):
- The $K$ centroids $\left(\boldsymbol{\mu}_{1}, \ldots \boldsymbol{\mu}_{K}\right)$ in $p$-dimensional input space span a subspace of rank $K-1$, denote this subspace as $H$
- For any point $x$, we can project it onto $H$, and perform LDA on this reduced space
- Example 2 (PCA)
- Perform PCA on the entire data, and take the first several eigen-vectors as the subspace $H$


## Discriminant Coordinates

Linear Discriminant Analysis


FIGURE 4.4. A two-dimensional plot of the vowel training data. There are eleven classes with $X \in \mathbb{R}^{10}$, and this is the best view in terms of a LDA model (Section 4.3.3). The heavy circles are the projected mean vectors for each class. The class overlap is considerable.

## Discriminant Coordinates



FIGURE 4.11. Decision boundaries for the vowel training data, in the two-dimensional subspace spanned by the first two canonical variates. Note that in any higher-dimensional subspace, the decision boundaries are higher-dimensional affine planes, and could not be represented as lines.

## Discriminant Analysis in Large $p$ problems

- When $p$ is large, QDA/LDA may not be applicable, because $\widehat{\Sigma}^{-1}$ does not exist
- Using generalized inverse can easily overfit the data
- A warning sign: Classes are well-separated on the training data could be meaningless for high-dimensional data
- Regularization: sparse LDA, Naive Bayes, RDA


## Sparse LDA

- Witten and Tibshirani (2011): penalized LDA

$$
\underset{a}{\operatorname{maximize}}\left\{a^{\top} \mathbf{B} a+P(|a|)\right\} \quad \text { subject to } \quad a^{\top}(\mathbf{W}+\Omega) a=1
$$

where $\Omega$ is some matrix that makes $(\mathbf{W}+\Omega)$ positive definite, and $P(|a|)$ is a penalty function over the vector $|a|$.

- Another approach Clemmensen et. al. (2011): similar idea with a different objective function that makes the optimization problem easier.


## Regularized Discriminant Analysis (RDA)

- Friedman (1989): shrink the separate covariances of QDA toward a common covariance in LDA. Regularized covariance matrices are

$$
\widehat{\Sigma}_{k}(\alpha)=\alpha \widehat{\Sigma}_{k}+(1-\alpha) \widehat{\Sigma}
$$

- $\alpha \in[0,1]$, a continuum of models between LDA and QDA, if $\widehat{\Sigma}$ is the pooled covariance matrix used in LDA
- In practice, chose $\alpha$ using CV.
- We can further shrink $\Sigma_{k}$ towards the diagonal covariance, with $\gamma \in[0,1]$

$$
\widehat{\Sigma}_{k}(\alpha, \gamma)=\alpha \widehat{\Sigma}_{k}+(1-\alpha) \gamma \widehat{\Sigma}+(1-\alpha)(1-\gamma) \widehat{\sigma}^{2} \mathbf{I}
$$

## Naive Bayes

- Recall that the optimal decision rule is

$$
\underset{k}{\arg \max } \mathrm{P}(Y=k \mid X=x)=\underset{k}{\arg \max } \pi_{k} f_{k}(x)
$$

- We can approximate $f_{k}(x)$ by

$$
f_{k}(x) \approx \prod_{j=1} f_{k j}\left(x_{j}\right)
$$

meaning that each dimension of $x$ is approximately independently

- $f_{k j}\left(x_{j}\right)$ can be estimated using histograms (discrete), or kernel densities (continuous)

Remarks

## Logistic Regression vs. LDA

- For LDA, the log-posterior odds between class 1 and 0 are linear in $x$

$$
\begin{aligned}
\log \frac{\mathrm{P}(Y=1 \mid X=x)}{\mathrm{P}(Y=0 \mid X=x)}= & \log \frac{\pi_{1}}{\pi_{0}}-\frac{1}{2} \boldsymbol{\mu}_{1}^{\top} \Sigma^{-1} \boldsymbol{\mu}_{1}+\frac{1}{2} \boldsymbol{\mu}_{0}^{\top} \Sigma^{-1} \boldsymbol{\mu}_{0} \\
& +x^{\top} \Sigma^{-1}\left(\boldsymbol{\mu}_{1}-\boldsymbol{\mu}_{0}\right) \\
= & \alpha_{0}+x^{\top} \boldsymbol{\alpha}
\end{aligned}
$$

- Logistic model has linear logics by construction

$$
\log \frac{\mathbf{P}(Y=1 \mid X=x)}{\mathbf{P}(Y=0 \mid X=x)}=\beta_{0}+x^{\top} \boldsymbol{\beta}
$$

- Are they the same estimators?


## Logistic Regression vs. LDA

- For LDA, the The linearity is a consequence of the Gaussian assumption for the class densities, and the assumption of a common covariance matrix.
- For logistic regression, the linearity comes by construction.
- The difference lies in how the coefficients are estimated.
- Which is more general?
- LDA assumes Gaussian distribution of $X$; while logistic leaves the density of $X$ arbitrary
- Logistic model is more general


## R Functions

- LDA and QDA: R package MASS, functions lda, qda.
- Logistic: R function glm
- General optimization: R function optim

